Chemical Physics Letters 708 (2018) 188–193

Contents lists available at ScienceDirect

Chemical Physics Letters

journal homepage: www.elsevier.com/locate/cplett

Research paper

# A new antimony carbide monolayer: An indirect semiconductor with a tunable band gap

M.M. Abutalib*

*Department of Physics, Faculty of Science, University of Jeddah, Jeddah, Saudi Arabia*
*Department of Physics, Faculty of Science-AL Faisaliah Campus, King Abdulaziz University, P.O. Box. 80200, Jeddah 21589, Saudi Arabia*

## HIGHLIGHTS

- A new stable antimony carbide monolayer is predicted.
- The predicted monolayer is **thermodynamically, kinetically, and thermally** is stable.
- $Sb_2C$ monolayer has an indirect band gap of 0.90 eV (1.45 eV) by using PBE (HSE06) level of theory.
- The electronic and optical properties of the $Sb_2C$ monolayer can be effectively engineered by strain effect.

## ARTICLE INFO

*Keywords:*
First principles calculation
Density functional theory
$Sb_2C$ monolayer
Indirect semiconductor

## ABSTRACT

To predict new materials with special electronic and optical properties can be considered as an effective procedure to design new potential applications. In this article by using density functional theory (DFT), a new two-dimensional structure of antimony carbide is theoretically predicted. Our DFT based simulations show that the proposed monolayer is energetically, kinetically, and thermally stable. By more investigation on its physical properties it is found that the $Sb_2C$ monolayer is an indirect semiconductor with interesting electronic and optical properties can be effectively modulated by biaxial external strains and has potential applications in new electronics technology.

## 1. Introduction

Since the discovery of the graphene [1], in the last decade, two-dimensional nanostructures have found a unique location in nanotechnology applications. Because of their unique properties such as high surface area, good synthesis conditions, controlling on their properties, etc, two dimensional materials can be used in many electronic and optical properties [2–19].

In 2014, a new two dimensional structure of carbon called penta-graphene or penta-carbon was proposed from first principles calculation [20]. Inspired by the predicting of the penta-graphene, in recent years, a number of new pentagonal 2D nano structures have been theoretically predicted [21–30]. A new stable two dimensional inorganic material called pentagonal $B_2C$ monolayer [21] was predicted by Li et al in 2015. It has been shown that the proposed penta-$B_2C$ is an indirect band gap semiconductor with a band gap of about 2.28 eV (calculated by PBE0) can be effectively tuned by strain effect [22]. Afterwards, another 2D monolayer with a similar pentagonal structure of carbon-nitride with a chemical formula of $CN_2$, indicates an insulating nature has been proposed by Zhang et al., in 2016 [23]. Furthermore, more recently, by using first principles calculations based on density functional theory, a number of new two dimensional semiconductors named $As_2C$ monolayer [24], penta-$CdS_2$ [25], penta-$Sb_2Si$ [26], penta-$SiC_5$ [27], penta-$P_2X$ (X = C, Si) [28], penta-$XP_5$(X = Al, Ga, In) [38] with a similar pentagonal structure have been theoretically reported.

In all of these two dimensional materials, a unit cell is formed by six atoms which are located in three different planes; two four-coordinated atoms at the middle plane and four three-coordinated locate at the two outer planes. As an example, in a unit cell of the there are four three-coordinated carbons with $sp^3$- and two four-coordinated carbons with $sp^2$-hybridyzation, forming a network of atoms in three different planes.

In continue to the proposing of the abovementioned monolayer structures, in this paper, using the first principles calculations in the framework of the density functional theory a new pentagonal monolayer namely antimony carbide monolayer is predicted.

* Address: Department of Physics, Faculty of Science, University of Jeddah, Jeddah, Saudi Arabia.
*E-mail address:* mabotaleb@uj.edu.sa.

https://doi.org/10.1016/j.cplett.2018.08.020
Received 1 July 2018; Accepted 4 August 2018
Available online 10 August 2018

## 2. Computational methods and details

To find fully relaxed ground state of the proposed monolayer, a joint atomic coordinate relaxation as well as lattice optimization procedures was used by using the density functional perturbation theory (DFPT) implemented in QUANTUM ESPRESSO package [30], where the Troullier-Martins norm-conserving psedupotential is considered to treat the core electron [31]. Also, the valance electrons wave functions are expanded by using energy cut off of 60 Ry.

The stability of the designed structure was confirmed by employing three procedures, the cohesive energy calculation, the phonon evaluation, and the first-principles molecular dynamics simulation.

The thermodynamic stability by calculating its cohesive energies ($E_{coh}$), where cohesive energy is defined as

$$E_{coh} = (4E_{Sb} + 2E_C - E_{Sb2C})/6. \quad (1)$$

To confirm the thermal stability, a first-principles molecular dynamics simulation in the canonical ensemble (NVT) was performed by employing the DMOL3 code [32].

When investigating electronic and optical properties, the density functional theory based full potential linear augmented plane waves plus local orbital (FPLAPW + lo) first-principles calculation implemented in WIEN2k code [33] is employed. The exchange-correlation potential was treated with the generalized gradient approximation parameterized by the Perdew Burke Ernzerhof functional (GGA-PBE) [34]. To gain the complex dielectric function components, the random phase approximation (RPA) method and the Kramers-Kronig relations are employed, where Gaussian broadening of 0.2 eV was applied. Based on Monkhorst-Pack approximation [35], the first Brillouin zone (BZ) was sampled by 10×10×1 and 20×20×1 k-mesh for electronic and optical calculations, respectively. The input parameters of $R_{MT}Kmax = 7$, $Gmax = 14\ Ry^{1/2}$ and $lmax = 10$ were used. Also, to avoid neighboring layers interactions, a vacuum layer of 15 Å in non-periodic direction (z-axis) is considered.

## 3. Optimized ground state properties

### 3.1. The ground state properties of the $Sb_2C$ monolayer

At the first step, it is needed to find the optimized ground state structure of the possible stable $Sb_2C$ monolayer and check its stabilities. By replacing the four $sp^3$-hybridyzation carbons of the penta-graphene with antimony atoms, a possible unit cell of the $Sb_2C$ monolayer is achieved. To find the optimized lattice parameters of the ground state of the predicted structure, its total energy versus its volume was calculated by using Brich-Murnaghan thermodynamic equation state [36];

$$E(V) = E_0 + \frac{9B_0V_0}{16}\left\{\left[\left(\frac{V_0}{V}\right)^{2/3} - 1\right]^3 \overset{\text{Å}}{B_0}\right\} + \frac{9B_0V_0}{16}\left\{\left[\left(\frac{V_0}{V}\right)^{2/3} - 1\right]^2\left[6 - 4\left(\frac{V_0}{V}\right)^{2/3}\right]\right\}, \quad (2)$$

In this equation, $V_0$, $V$, $B_0$, $\overset{\text{Å}}{B_0}$ are the initial considered volume, deformed volume, bulk modulus, and derivative of the bulk modulus with respect to pressure. Needles to say, the minimum point of the E-V curve provides the equilibrium lattice constant of the crystal cell. According to Fig. 1(c), the optimized lattice constant is calculated as a = b = 4.83 Å.

A 4×3 super cell of the predicted monolayer is presented in Fig. 1(a), by a closer look at the Fig. 1(a), it is seen that a unit cell of the monolayer contains four three-coordinated antimony and two four-coordinated carbon atoms. Each carbon atom bonds with its four neighboring antimony atoms and each antimony atom bonds with two carbon atoms and an antimony atom, forming a buckled pentagonal network with a buckling thickness of 2.81 Å. For the optimized structure, the lengths of 2.97 Å, and 2.21 Å are calculated for Sb-Sb and Sb-C bonds, respectively. Furthermore, the calculation shows that the angles of Sb-Sb-C, Sb-C-Sb, and C-Sb-C are$95.\dot{5}78$, $101.\dot{3}89$, and $100.\dot{2}78$ degree respectively. The atomic coordinate's information of the optimized $Sb_2C$ monolayer is given in Table1.

### 3.2. Stability of the predicted monolayer

The thermodynamic stability of the predicted structure was evaluated by calculating its cohesive energies ($E_{coh}$). When using this definition presented in Eq. (1), our calculation shows that the monolayer exhibits a cohesive energy of 4.45 eV/atom. By comparing the obtained cohesive energy with those for graphene [1] (7.94 eV/atom), T-Carbon [37] (6.67 eV/atom), silicene [5] (3.94 eV/atom) and phsophorene [38] (3.44 eV/atom) which are obtained by using same method, one can conclude that the predicted monolayer has a good thermodynamic stability. It is worth pointing out that the cohesive energy cannot directly describe the relative stability of different structures, but the calculated cohesive energy can be considered as clear evidence that the proposed monolayer is strongly bonded.

Then the kinetic stability of the proposed monolayer was confirmed by calculating its phonon bands. In this computation the density functional perturbation theory (DFPT) implemented in QUANTUM ESPRESSO package was used. Fig. 2 (left panel) shows the phonon dispersion curves of the proposed monolayer, in which, the absence of imaginary modes in the entire Brillouin zone confirms that the predicted structure is dynamically stable. Furthermore, the highest calculated frequency for the monolayer is 622/cm which is higher than the highest frequency of 580/cm for silicone [5], and 473/cm for $MoS_2$ [39].

As the last stability evaluation, the thermal stability of the structure was checked by performing first-principles molecular dynamics (FPMD) simulations. In this simulation, a 3×3×1 super-cell was considered and an MD simulation was carried out for the monolayer at temperatures of 500 K for 10 ps heating, where, the simulation reveals that the monolayer retains its structure at the temperatures of 500 K at the end of 10 ps heating, indicates that the $Sb_2C$ monolayer exhibits a good thermal stability. Fig. 2 (right panel), presents top and side views of snapshots of $Sb_2C$ monolayer at the end of 10 ps MD simulation at 500 K.

Although the predicted $Sb_2C$ monolayer indicates good stability, it only proves it is a local minimum structure. Since global minimum structures have more possibility to be realized experimentally, one may check if our obtained $Sb_2C$ monolayer is the global minimum structure in 2D space by using a series of approaches of materials design protocols, such as USPEX1, CALYPSO, AMADEUS, XtalOpt, or AIRSS [40–43]. However, since the previously predicted 2D materials exhibit this atomic configuration such as penta-graphene [20] and B2C monolayer [21], they are meta-stable compared to their global minimum counterparts, the global minimum search procedure has not preform here.

## 4. Electronic properties

The calculated band structure, and density of states of the $Sb_2C$ monolayer along the directions with the highest symmetry in Brillouin zone is shown in Fig. 3. According to Fig. 3, the predicted $Sb_2C$ monolayer is a semiconductor with an indirect band gap of about 0.90 eV. Moreover, the valance band maximum of the band structure is located somewhere between X and Γ points, and the conduction band minimum is located at Γ point. As seen in Fig. 3, the both p orbitals of the antimony and carbon atoms have considerable contribution in the top of the valence band (VB) and the bottom of the conduction band (CB). However, the p orbital of the carbon atom makes a more important role in the electronic bands around the Fermi level, which is due to the higher electron negativity of carbon (2.55) than the electron negativity of antimony (2.05). Since GGA-PBE theory commonly results